

Advanced Polymer Materials for Batteries

Project ID: bat555

PI/Co-PI: Zhenan Bao (Stanford, SLAC)/Yi Cui (Stanford, SLAC)

Objective: Explore the rational polymer materials design to effectively suppress the dendrite growth, control volume change and manage side reactions related to lithium metal charge/discharge processes. This will lead to development of next generation high-energy, low-cost batteries for electric vehicles

Impact:

- Improve cycling stability, Coulombic efficiency and current density of lithium metal anode
- Enable high-energy lithium-metal batteries for electric vehicles and reduce cost of batteries

Accomplishments:

- Design and synthesize a series of self-healing polymers (SHPs) with adaptive mechanical property
- Show the Li metal deposition morphology with self-healing polymer as protection layer
- Establish systematic understanding for polymer coating design and demonstrate improved cycling life for Li metal under SHP protection
- Developed new polymer coating concept with cation-tethered flowable polymer interface and demonstrate enhanced performance

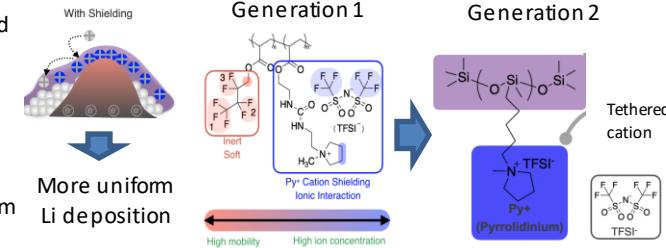
FY21 Milestones:

- Analyze new polymer chemistry and mechanical properties (Q1, completed)
- Analyze the stability of polymer coating in electrolyte and its protection of lithium metal surface (Q2, completed)
- Characterize the impact of the polymeric coating on lithium deposition morphology (Q3, completed)
- Complete evaluation of Li metal electrodes with the polymeric coating (Q4, completed)

Approach: We design flowable polymer coatings for uniform deposition/stripping of lithium metal and improved cycling stability of Li-metal electrodes.

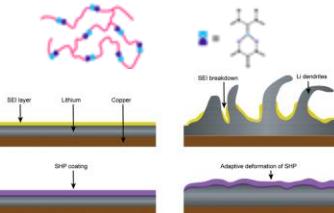
Funding: FY21: \$450,00, FY20: \$450,00, FY19: \$450,00

Key concept: A cation-tethered flowable polymeric interface for enabling stable deposition of metallic Li



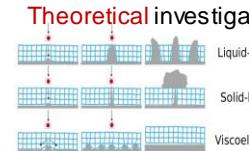
Z Huang*, S Choudhury*, H Gong, Y Cui, Z Bao, *JACS*, 2020
Z Huang*, J. Lai*, Y Cui, Z Bao, *paper in preparation*

A flowable artificial SEI for Li metal



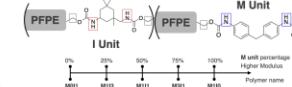
G. Zheng*, C. Wang*, A. Pei*, J. Lopez*, Y. Cui, Z. ACS Energy Lett. 1247–1255 (2016)
J. Lopez, Y. Cui, Z. Bao et al, *JACS* 2018

Effect of coating mechanics



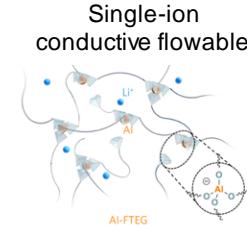
X. Kong, P. Rudnicki, S. Choudhury, Z. Bao, J. Qin, *Adv. Funct. Mater.* 2020, 1910138.

Theoretical investigation



Z. Huang, S. Choudhury, N. Paul, R. Gilles, Z. Bao, *Adv. Energy Mater.* (2021)

Effect of coating chemistry



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Zhenan Bao publication list in BMR

FY 20

1. D.T. Boyle, X. Kong, A. Pei, P.E. Rudnicki, F. Shi, W. Huang, Z. Bao, J. Qin, Y. Cui, "Transient Voltammetry with Ultramicroelectrodes Reveals the Electron Transfer Kinetics of Lithium Metal Anodes", **ACS Energy Lett.** 5, 701-709, 2020.
2. X. Kong, P. E. Rudnicki, S. Choudhury, Z. Bao, and Jian Qin, "Dendrite Suppression by a Polymer Coating: A Coarse-Grained Molecular Study", **Adv. Funct. Mater.**, 1910138, 2020.
3. Z. Huang, S. Choudhury, H. Gong, Y. Cui, and Z. Bao " A Cation-Tethered Flowable Polymeric Interface for Enabling Stable Deposition of Metallic Lithium " **JACS** (2020) DOI: 10.1021/jacs.0c09649
4. C. V. Amanchukwu, Z. Yu, X. Kong, J. Qin, Y. Cui, and Z. Bao. "A new class of ionically conducting fluorinated ether electrolytes with high electrochemical stability." **Journal of the American Chemical Society** 142, 7393-7403, 2020.
5. D. G. Mackanic, T.-H. Chang, X. Huang, Y. Cui, Z. Bao, "Stretchable electrochemical energy storage devices", **Chem. Soc. Rev.**, 49, 4466-4495, 2020.
6. D. G. Mackanic, M. Kao, Z. Bao, "Enabling Deformable and Stretchable Batteries", **Adv. Energy Mater.**, 10, 2001424, 2020
7. Z. Yu, H. Wang, X. Kong, W. Huang, Y. Tsao, D.G. Mackanic, K. Wang, X. Wang, W. Huang, S. Choudhury, Y. Zheng, C. Amanchukwu, S.T. Hung, Y. Ma, E.G. Lomeli, J. Qin, Y. Cui, Z. Bao, "Molecular design for electrolyte solvents enabling energy-dense and long-cycling lithium metal batteries", **Nature Energy**, 5, 526-533, 2020.
8. Z. Yu, Y. Cui, Z. Bao, "Design principles of artificial solid electrolyte interphases for lithium-metal anodes", **Cell Rep. Phys. Sci.**, 1, 100119, 2020.

Zhenan Bao publication list in BMR

FY 21

1. D.T. Boyle, W. Huang, H. Wang, Y. Li, H. Chen, Z. Yu, W. Zhang, Z. Bao, Y Cui, "Corrosion of lithium metal anodes during calendar ageing and its microscopic origins" **Nature Energy** 6, 5, pg 487-494, 35, 2021.
2. H. Wang, W. Huang, Z. Yu, W. Huang, R. Xu, Z. Zhang, Z. Bao, Y. Cui, "Efficient Lithium Metal Cycling over a Wide Range of Pressures from an Anion-Derived Solid-Electrolyte Interphase Framework" **ACS Energy Letters** 6, 2, pg 816-825, 14, 2021.
3. J. Li, Y. Cai, H. Wu, Z. Yu, X. Yan, Q. Zhang, T.Z. Gao, K. Liu, X. Jia, Z. Bao, "Polymers in Lithium-Ion and Lithium Metal Batteries" **Advanced Energy Materials** 11 (15), 2003239, 26, 2021.
4. S.C. Kim, X. Kong, R.A. Vilá, W. Huang, Y. Chen, D.T. Boyle, Z. Yu, H. Wang, Z. Bao, J. Qin, Y. Cui, "Potentiometric measurement to probe solvation energy and its correlation to lithium battery cyclability", **Journal of the American Chemical Society** 143, 27, pg 10301-10308, 7, 2021.
5. H. Wang, Z. Yu, X. Kong, W. Huang, Z. Zhang, D.G. Mackanic, X. Huang, J. Qin, Z. Bao, Y. Cui, "Dual-Solvent Li-Ion Solvation Enables High-Performance Li-Metal Batteries", **Advanced Materials**, 2008619, 17, 2021.
6. Y. Chen, Z. Yu, P. Rudnicki, H. Gong, Z. Huang, S.C. Kim, J.C. Lai, X. Kong, J. Qin, Y. Cui, Z. Bao, "Steric effect tuned ion solvation enabling stable cycling of high-voltage lithium metal battery", **Journal of the American Chemical Society**, 143, 44, pg 18703-18713, 2, 2021.
7. Z. Huang, S. Choudhury, N. Paul, J.H. Thienenkamp, P. Lennartz, H. Gong, P. Müller-Buschbaum, G. Brunklaus, R. Gilles, Z. Bao, "Effects of Polymer Coating Mechanics at Solid-Electrolyte Interphase for Stabilizing Lithium Metal Anodes" **Advanced Energy Materials**, 2103187, 2021.
8. Y. Tsao, H. Gong, S. Chen, G. Chen, Y. Liu, T.Z. Gao, Y. Cui, Z. Bao, "A Nickel-Decorated Carbon Flower/Sulfur Cathode for Lean-Electrolyte Lithium–Sulfur Batteries", **Advanced Energy Materials** 11, 36, 2101449, 1, 2021.
9. X. Gao, X. Zheng, Y. Tsao, P. Zhang, X. Xiao, Y. Ye, J. Li, Y. Yang, R. Xu, Z. Bao, Y. Cui, "All-Solid-State Lithium–Sulfur Batteries Enhanced by Redox Mediators", **Journal of the American Chemical Society**, 143, 43, pg 18188-18195, 2021.

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FY 22

- Z.Yu, P.E. Rudnicki, Z. Zhang, Z. Huang, H. Celik, S.T. Oyakhire, Y. Chen, X. Kong, S. Kim, X. Xiao, H. Wang, Y. Zheng, G.A. Kamat, M. Kim, S.F. Bent, J. Qin, Y.Cui, Z.Bao, “Rational solvent molecule tuning for high-performance lithium metal battery electrolytes”. **Nat Energy** 7, 94–106, 2022.
- M.S. Kim, Z. Zhang, P.E. Rudnicki, Z. Yu, J. Wang, H. Wang, S.T. Oyakhire, Y. Chen, S.C. Kim, W. Zhang, D.T. Boyle, X. Kong, R. Xu, Z. Huang, W. Huang, S.F. Bent, L. Wang, J. Qin, Z.Bao, Y.Cui, “Suspension electrolyte with modified Li⁺ solvation environment for lithium metal batteries”. **Nat. Mater.** 21, 445-454, 2022.
- H.Wang, Z.Yu, X. Kong, S. Kim, D.T. Boyle, J. Qin, Z. Bao, Y. Cui, Y., “Liquid electrolyte: The nexus of practical lithium metal batteries”, **Joule**, 6, 588-616, 2022.
- Z. Zhang, Y. Li, R. Xu, W. Zhou, Y. Li, S.T. Oyakhire, Y. Wu, J. Xu, H. Wang, Z. Yu, D.T. Boyle, W. Huang, Y. Ye, H. Chen, J. Wan, Z. Bao, W. Chiu, Y. Cui, “Capturing the swelling of solid-electrolyte interphase in lithium metal batteries”. **Science**, 375, 66-70, 2022.